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Macromolecular Calculations in the XTAL System of Crystallographic Programs
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12 PERSONAL AUTHOR(S)
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			Macromolecular crystal structure analysis, computer codes for macromolecular crystals, Macromolecular Crystallographic Computing.

19 ABSTRACT (Continue on reverse if necessary and identify by block number)

This project is concerned with the production of crystallographic computer codes for the solution and refinement of macromolecular crystal structures. The computer programs are being prepared within the context of an existing suite of crystallographic computer programs called "XTAL".

Extensive documentation and testing is being done in addition to the programming.

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DATE: 27 June 1988

PROGRESS REPORT ON CONTRACT N00014-88-K-0323

PRINCIPAL INVESTIGATOR: James M. Stewart

CONTRACTOR: University of Maryland - Code 07419

CONTRACT TITLE: Macromolecular Calculations in the XTAL System of Crystallographic Programs

START DATE: 1 June 1988

RESEARCH OBJECTIVE: To produce, within the XTAL system, programs, documentation and tests for macromolecular crystallographic calculations.

PROGRESS (Since September 1987 in collaboration with D. M. Collins and K. B. Ward at the Naval Research Laboratory - Code 6030): In this period five programs for macromolecular calculations have been worked on.

1) MEDENS: A program which computes the constrained exponential density distribution corresponding to a lower resolution input Fourier electron density map. Given an input electron density map, the density is processed to give the exponential density distribution. This is a function of the maximum entropy and is intended to be used for the extropolation; interpolation and smoothing of reflection phases. The resulting phases must be recovered using the XTAL program RFOURR (completed in 1987). Extensive testing and documentation have been prepared.

2) MEFFIT: A program which computes a maximum-entropy electron density distribution of improved agreement with observed structure moduli. Given an input positive-definite electron density map produced by MEDENS and a difference electron density map based on calculated structure factors from its reverse Fourier transform, this program finds a new maximum-entropy map in better agreement with the observed structure factor amplitudes. Extensive testing and documenation have been prepared.

3) RMAP: A program to calculate 1/R or F_o*F_c correlation maps as a function of translation of a fragment of a structure in the crystal unit cell. This is an adaptation of a code produced outside the XTAL system by Dr. W. Furey at the Veterans Administration Medical Center in Pittsburg. Extensive testing and documentation have been prepared.

4) PROTIN: A program to read "constraint information" to describe the elements of a macromolecular crystal structure. This information, for example, can be the idealized coordinates for all the amino acids. This program is a translation of the Hendrickson-Konnert program by the same name. The XTAL version is coded and checked to some extent and preliminary documentation has been prepared.

5) PROLSQ: A program to do constrained least-squarers refinement of the positional and thermal parameters of a macromeolecular structure. This program is a translation into XTAL of the Konnert-Hendrickson program by the same name. The XTAL version is coded and at the present date checkout has begun.

WORK PLAN: In the coming year the greatest effort will be to bring PROTIN and PROLSQ to fully checked out status and full documentation. In addition, PROLSQ must be altered to use a fast Fourier transform approach which will enhance computing times.

Futher programs planned for the future are the translation and systematization of B.C. Wang's; for example: ENVLOP, which produces a smoothed low resolution electron density map. A program to produce electron density maps about any origin from a conventional map, and enhancement of the MEDENS/MEFFIT programs recently completed so that it will be more straightforward for the user to run maximum-entropy calculations.

PUBLICATIONS AND REPORTS:

1. XTAL User's Manual, Editors Hall & Strewart, Version 2.4 May 1988.

2. Electron densities from limited phase information by entropy maximization, D. M. Collins, Laboratory for the Structure of Matter, Naval Research Laboratory, Washington, D.C. 20375, J. M. Stewart, Department of Chemistry and Biochemistry, University of Maryland, College Park, MD 20742 at the European Crystallographic Conference in Vienna-Austria, August 1988.

SUMMER STUDENT: A student helper is being supported in Summer 1988 to begin the translation of the B.C. Wang codes to XTAL.

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Minorities	- 0
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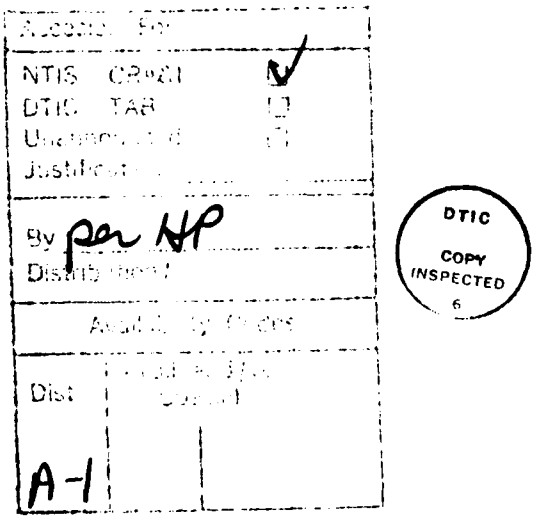

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